ISSN 0018-151X, High Temperature, 2018, Vol. 56, No. 2, pp. 201–207. © Pleiades Publishing, Ltd., 2018.
Original Russian Text © R.M. Khusnutdinoff, A.V. Mokshin, A.L. Bel'tyukov, N.V. Olyanina, 2018, published in Teplofizika Vysokikh Temperatur, 2018, Vol. 56, No. 2, pp. 211–218.

THERMOPHYSICAL PROPERTIES OF MATERIALS

Viscosity of Cobalt Melt: Experiment, Simulation, and Theory

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Received December 23, 2016

Abstract—The results of experimental measurements, molecular dynamics simulation, and theoretical calculations of the viscosity of a cobalt melt in a temperature range of 1400–2000 K at a pressure $p = 1.5$ bar corresponding to an overcooled melt at temperatures of 1400–1768 K and an equilibrium melt with temperatures from the range 1768–2000 K are presented. Theoretical expressions for the spectral density of the time-dependent correlation function of the stress tensor $\tilde{S}(\omega)$ and kinematic viscosity ν determined from the frequency and thermodynamic parameters of the system are obtained. The temperature dependences of the kinematic viscosity for the cobalt melt are determined experimentally by the torsional oscillation method; numerically, based on molecular simulation data with the EAM potential via subsequent analysis of the time correlation functions of the transverse current in the framework of generalized hydrodynamics; and by the integral Kubo–Green relation; they were also determined theoretically with the Zwanzig–Mori memory functions formalism using a self-consistent approach. Good agreement was found between the results of theoretical calculations for the temperature dependence of the kinematic viscosity of the cobalt melt using experimental data and the molecular dynamics simulation results. From an analysis of the temperature dependence of the viscosity, we obtain an activation energy of $E = (5.38 \pm 0.02) \times 10^{-20}$ J.

DOI: 10.1134/S0018151X18020128

INTRODUCTION

Amorphous-forming fluids that do not crystallize upon cooling and retain a disordered structure down to very low temperatures are a subject of intensive research in condensed matter physics [1–4]. A specific feature of such systems is associated with the temperature dependence of the viscosity (or the structural relaxation time), which varies by more than 15 orders of magnitude when passing from the liquid to the amorphous phase [5]. Amorphous metallic alloys (AMAs) are of particular interest, since they have unique physicomechanical properties [6–10]. Typically, AMAs are a multicomponent system with a high glass-forming ability that forms an amorphous phase at cooling with the rates $\gamma = (10^4–10^7)$ K/s [11, 12]. As shown in numerous molecular dynamics studies [13–19], an amorphous phase can also be obtained in the case of one-component (pure) metals as a result of superfast quenching ($\gamma = 10^{11}–10^{13}$ K/s). It is noteworthy that ferromagnetic transition metals (Fe, Ni, and Co), which are widely used in the aerospace industry, represent a particular case of single-component glass-forming metallic systems [7, 8, 20]. In this case, cobalt, as compared with iron and nickel, remains poorly understood. Thus, in particular, problems related to transport processes (self-diffusion, viscosity, thermal conductivity, and electrical conductivity) and the mechanisms by which collective excitations propagate in an equilibrium liquid and supercooled cobalt phases are unclear. This is partially due to the lack of experimental viscosimetry, inelastic X-ray, and neutron scattering data for this substance [20, 21]. The known experimental data on the viscosity of equilibrium liquid cobalt obtained by different researchers [22] reveal a significant (above 30%) discrepancy, which indicates the need for further research to clarify the absolute values of viscosity. Note that no viscosity values of the supercooled cobalt melt are currently found in the scientific literature.

This paper discusses the results of experimental measurements and molecular dynamics calculations of the viscosity of a cobalt melt in equilibrium liquid and supercooled phases. The kinematic viscosity was determined for the domain above and below the melting point $T_m(\mathrm{Co}) = 1768$ K: in the experiment for the temperature range $T = 1506–1969$ K and in simulation for 1400–2000 K.

EXPERIMENTAL

Experimental measurements were carried out for cobalt metal grade K0, which has a weight fraction of cobalt of at least 99.98% and contains the following impurities: 0.003% of Fe; less than 0.005% of Ni and C;